Improved numerical technique to calculate statistical Coulomb blurring

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This paper studies the effects of Coulomb blurring in charged-particle optics using a method that combines Monte Carlo techniques with analytical calculations. A correction factor for the analytical theory of Jansen and Kruit is obtained. This approach strongly enhances the accuracy of the method, while maintaining the speed of calculation. The method gives good agreement with Monte Carlo simulations. The effects of aperturing are also included.
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I. INTRODUCTION

The calculation of statistical Coulomb interactions in charged-particle optical systems has been a long-standing problem.[1–7] One can roughly distinguish two approaches: analytical calculations and Monte Carlo simulations.[8] In Monte Carlo simulations, one takes a sample of particles with random initial conditions (although satisfying the beam characteristics). The trajectories of these particles are then numerically evaluated as they go through the column. Although straightforward, the calculations are often time consuming and are usually not performed in the actual design process. Analytical approaches are much faster, but they usually rely on a number of assumptions needed to obtain analytical results in certain limits. One of the most extensive theories on Coulomb blurring is that of Jansen.[4] Here the values for the Coulomb interaction are based on analytical results obtained for the limits $r_{\mathrm{beam}} \to 0$ and ∞, where r_{beam} is the beam radius. Values for the Coulomb interaction for intermediate r_{beam} values are obtained via interpolation. It was already noted[4,5] that especially in the intermediate regime deviations exists. One of the reasons for these deviations is the fact that the Coulomb interactions are calculated for on-axis trajectories, whereas the statistical Coulomb forces could be different off axis. With the advances in charged-particle optics and the use of brighter sources, Coulomb blurring becomes increasingly a limiting aberration. For example, for standard Ga liquid-metal-ion-source columns,[9] Coulomb blurring is estimated to be the largest or second-largest aberration over the current range from 1 pA to 1 μA. For many applications the column is run in the intermediate regime, where the largest deviations are expected. In order to obtain more reliable estimates of the Coulomb blurring, we show here how numerical Monte Carlo like results can be incorporated in an analytical calculation. This approach strongly enhances the accuracy of the method, while maintaining the speed of calculation.

The paper is organized as follows. We start with a brief explanation of the analytical calculation of Coulomb blurring. We then show how to incorporate Monte Carlo like results into the analytical approach. We also include the effects of aperturing. We end with the conclusions.

II. STATISTICAL COULOMB INTERACTIONS

When dealing with Coulomb forces in charged-particle optics, one often divides the interaction into two components: the longitudinal one, which affects the particle along the optical axis, causes a change in the kinetic energy leading to chromatic effects (this is usually known as the Boersch effect[1]), and the radial component of the particle's position, perpendicular to the optical axis, which gives rise to trajectory displacements.[2] In this article we focus on the latter since the former can often be effectively included in the intrinsic energy spread of the source. For the radial component of the particle position, we are interested in dr/dz resulting from the effective Coulomb force F_r^{blur} acting on the particle. The change in r is determined by Newton's law, given by

$$r'' = \frac{d^2 r}{dz^2} = \left(\frac{dt}{dz}\right)^2 \frac{d^2 r}{dt^2} = \frac{1}{m v_z^2}\left(F_r^{\mathrm{e.s.}} + F_r^{\mathrm{blur}}\right), \tag{1}$$

where $F_r^{\mathrm{e.s.}}$ is the force due to the lens fields, which we take here to be electrostatic. Generally, the stochastic Coulomb forces are much smaller than $F_r^{\mathrm{e.s.}}$, and we therefore treat them as a perturbation. The unperturbed rays can be found from the usual ray equation[10]

$$r'' + \frac{V'}{2V} r' + \frac{V''}{4V} = 0, \tag{2}$$

where V is the axis potential. The general lowest-order trajectory can be written as a sum of two independent solutions of the ray equation,

$$r(z) = \alpha X(z) + \beta Y(z), \tag{3}$$

where the boundary conditions for X and Y are given by $X(z_0)=0$, $X'(z_0)=1$ and $Y(z_0)=1$, $Y'(z_0)=0$, with z_0 the position of the virtual source. Thus, the physical interpretations of α and β are the half-beam opening angle at the source and the virtual source size, respectively.

The effect of statistical Coulomb interactions can be included by the method of variation of parameters. The effect

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of the Coulomb interactions in a thin beam slice at a certain position z can be taken into account by requiring that the trajectory is continuous,

$$d\alpha^{\mathrm{blur}}(z)X(z)+d\beta^{\mathrm{blur}}(z)Y(z)=0, \tag{4}$$

and that the change in trajectory is determined by the stochastic force in the radial direction working on the particle $r''_{\mathrm{blur}}=F_r^{\mathrm{blur}}/(mv_z^2)$,

$$d\alpha^{\mathrm{blur}}(z)X'(z)+d\beta^{\mathrm{blur}}(z)Y'(z)=r''_{\mathrm{blur}}(z). \tag{5}$$

From this set of equations, one easily obtains

$$d\beta^{\mathrm{blur}}(z)=-\frac{r''_{\mathrm{blur}}(z)X(z)}{X'(z)Y(z)-X(z)Y'(z)} \tag{6}$$

$$=-r''_{\mathrm{blur}}(z)X(z)\sqrt{V(z)/V_0}. \tag{7}$$

The total ray is then given by

$$r(z)=[\alpha+\alpha^{\mathrm{blur}}(z)]X(z)+[\beta+\beta^{\mathrm{blur}}(z)]Y(z), \tag{8}$$

with the coefficients

$$\beta^{\mathrm{blur}}(z)=\int_{z_0}^{z}d\tilde{z}\,d\beta^{\mathrm{blur}}(\tilde{z}), \tag{9}$$

and likewise for α^{blur}. The contribution of Coulomb blurring to the total spot size is now given by $r^{\mathrm{blur}}=M\beta^{\mathrm{blur}}(z_{\mathrm{foc}})$, where z_{foc} is the focal point and $M=Y(z_{\mathrm{foc}})$ the magnification.

The idea behind the analytical calculation of stochastic Coulomb interactions is finding a good estimate of F_r^{blur}. Since we are dealing with statistical quantities there is a probability distribution function of forces. The value that we shall use here is the median F_{r50}^{blur} of the force distribution function, where the a_{50} value for a probability function $\rho(a)$ in two dimensions is defined by

$$\int_0^{a_{50}}\rho(a)2\pi a\,da=\frac{1}{2}, \tag{10}$$

with $a=\sqrt{a_x^2+a_y^2}$. Thus the a_{50} value contains 50% of the probability distribution function. We prefer to use the F_{r50}^{blur} value instead of the full width at half maximum (FWHM) of the distribution function. The reason for this is that in certain limits the probability function becomes very narrow and the FWHM then gives a poor estimate of the forces working on the particle.

The next step is to derive the $r''_{50,\mathrm{blur}}$ values. Since speed of calculation is of importance, one does not like to calculate probability distribution functions too often. Jansen[4] uses for his $r''_{50,\mathrm{blur}}$ values an interpolation between exact results that can be obtained in the limits $r_{\mathrm{beam}}\to 0$ and ∞. The relevant parameters for the distribution function of forces are r_{beam} and the linear particle density

$$\lambda=\frac{I}{ev_z}=\sqrt{m/2e^3V}\,I, \tag{11}$$

where λ^{-1} gives the average distance between the particles in the z direction.

We now want to obtain an estimate of the force in the radial direction,

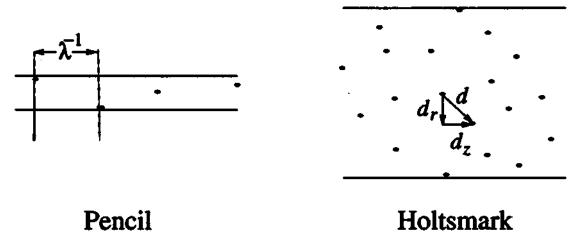

FIG. 1. Schematic presentation of the beam in the pencil and Holtsmark regimes. λ is the linear particle density.

$$F_r=\frac{e^2}{4\pi\varepsilon_0}\frac{d_r}{d^3}, \tag{12}$$

where d is the average particle distance and d_r the average distance in the radial direction. In the limit $r_{\mathrm{beam}}\to 0$ (often called the pencil regime; see Fig. 1), $d_r\to r_{\mathrm{beam}}$ and $d\to\lambda^{-1}$. For r''_{50P}, we find then

$$r''_{50P}=c_P\frac{m^{3/2}}{\varepsilon_0 e^{7/2}}\frac{I^3 r_{\mathrm{beam}}}{V^{5/2}}. \tag{13}$$

In the opposite limit, $r_{\mathrm{beam}}\to\infty$ (the Holtsmark regime; see Fig. 1), we have $d=\sqrt{2}d_r=\sqrt{2}d_z=(\pi r_{\mathrm{beam}}^2\lambda^{-1})^{1/3}$, giving

$$r''_{50H}=c_H\frac{m^{1/3}}{\varepsilon_0}\frac{I^{2/3}}{r_{\mathrm{beam}}^{4/3}V^{4/3}}. \tag{14}$$

Exact calculations[4] show that the constants are $c_P=0.435$ and $c_H=0.127$. Interpolation between the two different geometries is done according to[4]

$$\frac{1}{r''_{50A}}=\frac{1}{r''_{50H}}+\frac{1}{r''_{50P}}. \tag{15}$$

In a similar way, one can define the analytical value for the force as $F_{50A}=mv_z^2r''_{50A}$.

Although this interpolative scheme usually gives the right order of magnitude, it is quite often not accurate enough for design purposes. The major discrepancies occur in the intermediate region where r''_{50H} and r''_{50P} are of the same order of magnitude. A different approach to calculating Coulomb blurring is the use of Monte Carlo simulation. Here one takes a random bunch of particles that satisfy the desired beam characteristics and traces them through the column. This gives better results than the analytical method described above, but Monte Carlo calculations are generally time consuming and lack the ease of use of the analytical approach. The latter method can, however, be significantly improved by a better estimate of the r''_{50} value. In the remainder of the paper, we shall describe how this quantitity can be evaluated numerically and be incorporated as a correction factor into the analytical method.

III. NUMERICAL CALCULATION OF r''_{50}

To obtain the value of r''_{50}, one needs to determine the distribution functions of r''_{50} as a function of the distance to the optical axis r. This can be done by taking a cylinder with beam radius r_{beam} and of sufficient length l, i.e., long enough that finite size effects can be neglected (see Fig. 2). A probe

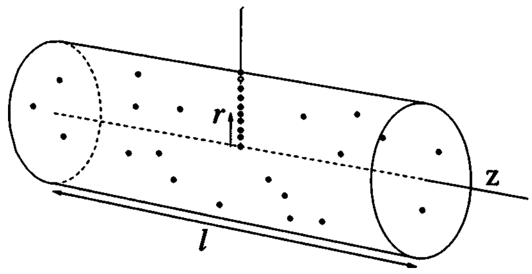

FIG. 2. Cylindrical beam used in the calculations of the force probability distribution functions. The cylinder with radius r_{beam} is filled randomly with particles corresponding to a certain linear particle density λ. The forces are then calculated for test particles that are placed in the middle of the cylinder at a distance r from the symmetry axis.

particle is then positioned in the middle of the cylinder at a distance r from the axis. The cylinder is then filled with particles of mass m corresponding to certain beam characteristics, i.e., λ and r_{beam}. The stochastic force on the probe particle $\mathbf{F}^{\mathrm{stoch}}$ is then calculated. Note that this force can be split into a longitudinal component $\mathbf{F}_{\parallel}^{\mathrm{stoch}}=F_z^{\mathrm{Boersch}}\hat{\mathbf{z}}$ and a perpendicular component $\mathbf{F}_{\perp}^{\mathrm{stoch}}$. This procedure is repeated until sufficient statistics has been obtained for the probability function of $\mathbf{F}_{\perp}^{\mathrm{stoch}}$. The probability distribution become almost independent of the number of particles for more than approximately 50–100 particles. (Calculations have been done with many more particles.) This shows that the statistical Coulomb force is mainly determined by interactions with particles that are close to the test particles.

Figure 3 shows typical probability distribution functions in the Holtsmark regime for the forces in the radial direction. We have used here $\lambda^{-1}=46\ \mu$m. For Ga ions, this corresponds to $V=30I^2$(nm) kV, for example, 30 kV and 1 nA. Calculations are done for $\lambda r_{\mathrm{beam}}=21.7$. We see two clear effects when moving away from the center toward the edge of the beam. First, we see that the probability function shifts due to the space charge effect. Secondly, the probability function becomes asymmetric. Figure 4 gives the probability distribution function of the radial forces in the pencil regime. A value for $\lambda r_{\mathrm{beam}}=0.11$ has been used. At the center of the beam the probability distribution function is a very narrow peak with long tails. For particles at the edge of the beam the distribution function has become strongly asymmetric. Note the absence of space charge effects.

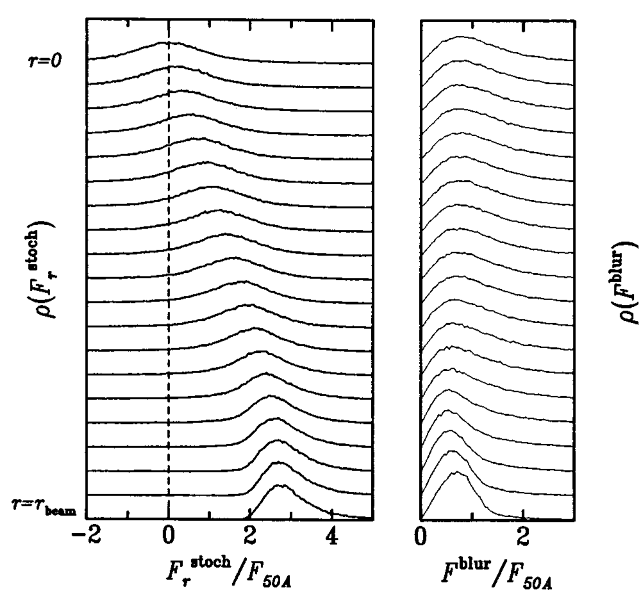

FIG. 3. Probability distributions of the Coulomb force on a particle at distance r from the center of the beam, on the left for the radial component, on the right for the absolute value after removal of the space charge effects. Calculations correspond to $\lambda r_{\mathrm{beam}}=21.7$. The actual calculations have been done for a beam with radius $r_{\mathrm{beam}}=1000\ \mu$m, filled with Ga ions with beam characteristics $V=30$ kV and $I=1$ nA.

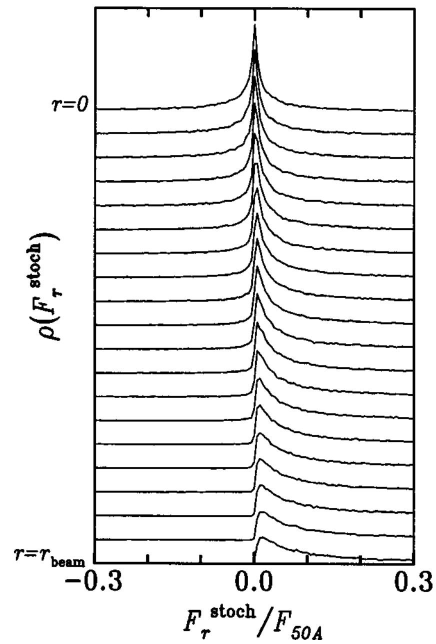

FIG. 4. Calculated probability distribution of the force as a function of distance to the symmetry axis under beam conditions $\lambda r_{\mathrm{beam}}=0.11$. The actual calculations have been done for a cylinder with a radius $r_{\mathrm{beam}}=0.1\ \mu$m filled with Ga ions using a current of $I=5$ nA and a beam voltage of 30 kV.

Since we are interested in the increase in spot size due to Coulomb blurring, we have to separate the effects from the space charge effects. For a homogeneous charge distribution the force as a result of space charge is

$$F_r^{\mathrm{space}}(r)=\frac{1}{2}\frac{en}{\varepsilon_0}r=N_e r, \tag{16}$$

where n is the charge density. Due to the proportionality to r, the effect of F_r^{space} is that of an ideal lens, leading to a defocusing. Since this does not directly lead to an increase in spot size we want to remove the r dependence, i.e., determine the constant N_e for a stochastic distribution. For a particular distance r from the optical axis we obtain

$$N_e(r)=\frac{1}{r}F_{r50}^{\mathrm{stoch}}(r), \tag{17}$$

where we use here the one-dimensional a_{50}, given by

$$\int_{-\infty}^{a_{50}}\rho(a)\,da=\frac{1}{2}, \tag{18}$$

where $\rho(a)$ gives the probability of finding quantity a. Thus 50% of the F_r^{stoch} is smaller and 50% of the F_r^{stoch} is greater

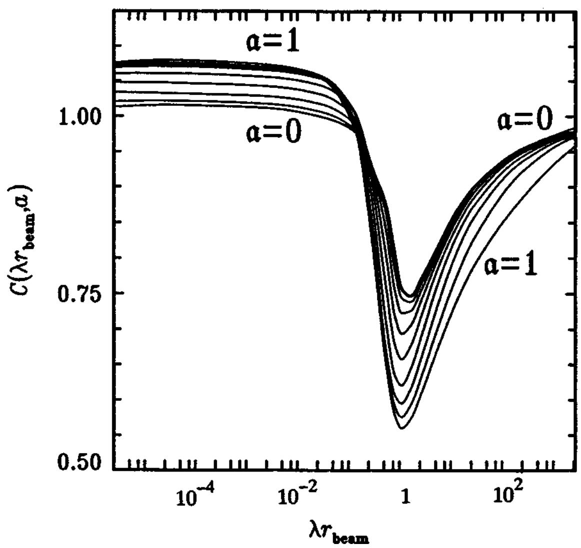

FIG. 5. The correction value $C(r_{\text{beam}},a)$ as a function of λr_{beam}. Curves are given for different aperture values a.

than $F_{r50}^{\text{stoch}}(r)$. Since there is one focus, we can use only one N_e for all r. We use here a weighted average of the $N_e(r)$:

$$\mathcal{N}_e(a)=\frac{1}{\pi(ar_{\text{beam}})^2}\int_0^{ar_{\text{beam}}}N_e(r)2\pi r\,dr. \tag{19}$$

We take into account here the effect of aperturing, by integrating not over the entire beam but only up to $r=ar_{\text{beam}}$ with $a\in[0,1]$, i.e., we calculate the effects on only the particles that actually contribute to the probe current.

Now, we define the Coulomb blurring force as the total stochastic force minus the space charge contribution, i.e.,

$$\begin{aligned}\mathbf{F}^{\text{blur}}(r)&=\mathbf{F}^{\text{stoch}}(r)-\mathbf{F}^{\text{space}}(r)\\&=[F_r^{\text{stoch}}-\mathcal{N}_e(a)r]\hat{\mathbf{r}}+F_\varphi^{\text{stoch}}\hat{\varphi}.\end{aligned} \tag{20}$$

The right side of Fig. 3 gives the probability function $\rho(F^{\text{blur}})$, where $F^{\text{blur}}=|\mathbf{F}^{\text{blur}}|$, using $\mathcal{N}_e(1)$. We clearly see a narrowing of the probability function for larger r, which indicates that the Coulomb blurring is less at the edge of the beam. From the probability function for a particular $r<ar_{\text{beam}}$, we can derive the $F_{50}^{\text{blur}}(r,a)$. The average $r''_{50,\text{blur}}$ is then given by

$$r''_{50,\text{blur}}(\lambda,r_{\text{beam}},a)=\int_0^{ar_{\text{beam}}}dr\,2\pi r\frac{F_{50}^{\text{blur}}(r,a)}{2\pi(ar_{\text{beam}})^2eV}. \tag{21}$$

This gives a correction factor to the original analytical r''_{50A} from Eq. (15),

$$C(\lambda r_{\text{beam}},a)=\frac{r''_{50}(\lambda,r_{\text{beam}},a)}{r''_{50A}}. \tag{22}$$

Note that, apart from the aperture constant a, $C(\lambda r_{\text{beam}},a)$ depends only on λr_{beam}. This can be understood as follows. Changing the values of r_{beam} and λ effectively corresponds to a renormalization of the r and z axes. When r and z are both scaled by a factor κ, the only thing that should happen to the radial Coulomb force $F_r=r/(r^2+z^2)^{3/2}$ is a renormalization by κ^{-2}. However, the forces F_{50P} and F_{50H} already scale this way. Therefore, distributions with equal λr_{beam} should have the same correction factor. The correction factors take into account the effects of a finite size of the beam and the different configurations of the particles with respect to each other off axis compared to on axis. Since the correction factor does not depend on m, I, V, and r_{beam}, but only on λr_{beam}, the calculational effort is strongly reduced. The function $C(\lambda r_{\text{beam}},a)$ can be simply tabulated and intermediate values can be interpolated.

Results for $C(\lambda r_{\text{beam}},a)$ are shown in Figs. 5 and 6. For $C(\lambda r_{\text{beam}},a)\to 1$ the analytical theory is valid. Note that substantial deviations are found in the intermediate region, where the interparticle distance d is comparable to the beam radius r_{beam}. Solving $r''_{50H}=r''_{50P}$ we find that the intermediate regime occurs for

$$\lambda r_{\text{beam}}=\frac{I}{ev_z}r_{\text{beam}}\cong 0.417, \tag{23}$$

whereas the minimum is found around $\lambda r_{\text{beam}}=1$. The correction is less for $a\to 0$, i.e., for particles close to the optical axis. Including particles at the edge of the beam in the probe forming current $(a\to 1)$ increases the deviations from the theory of Jansen.[4] Figure 6 shows the dependence on aperturing. In the Holtsmark regime, particles at the edge of the

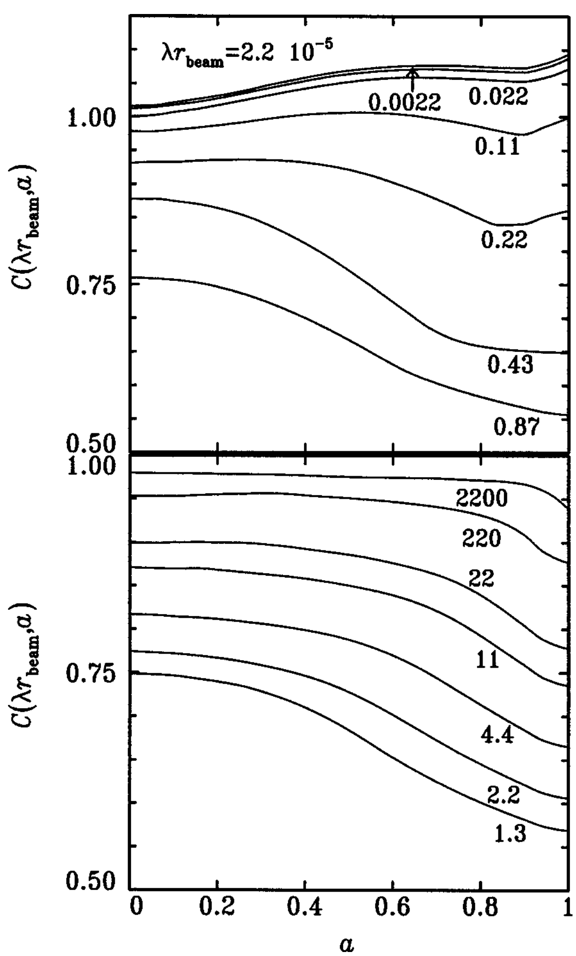

FIG. 6. The correction value $C(\lambda r_{\text{beam}},a)$ as a function of the aperture parameter a. Curves are given for different λr_{beam}.

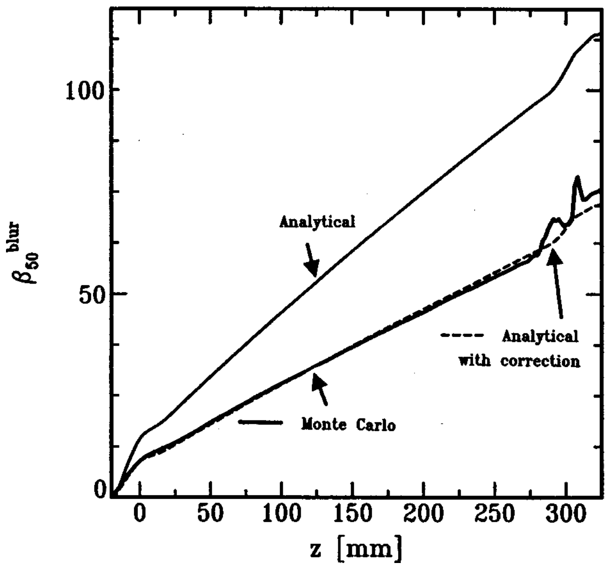

FIG. 7. Comparison between $\beta_{50}^{\mathrm{blur}}$ obtained using Monte Carlo, analytical (theory of Jansen), and corrected analytical calculations.

beam have a narrower probability function than particles in the center of the beam. A physical explanation for this is that at the edge of the beam there are mainly statistical interactions in one direction, thereby narrowing the probability distribution. In addition to that the distribution also becomes asymmetric (see Fig. 3). In the pencil regime the distribution becomes wider when $r \rightarrow r_{\mathrm{beam}}$. In this regime, the interactions are mainly in the longitudinal direction. Forces in the radial direction are determined by the angle $d_r\lambda$. For a particle on the axis the maximum d_r is equal to r_{beam}. However, for a particle at the edge of the beam, the maximum d_r can be twice as large (see Fig. 1). This results in larger F_r.

Figure 7 shows a comparison of Monte Carlo simulations with analytical calculations with and without correction. The Monte Carlo calculations were done using a fast-tree algorithm for calculating the Coulomb interactions[11] and a fifth-order Runge-Kutta integration method with variable step size.[12] In the Monte Carlo method the difference from the unperturbed trajectories is $\Delta\mathbf{r}_i(z)$. However, this quantity is not very useful in estimating what the final spot size will be. More information can be obtained by separating the value of $\beta_{i\eta}$, where $\eta = x,y$, by

$$\beta_{i\eta}^{\mathrm{stoch}}(z) = -\frac{\Delta\eta'(z)X(z) - \Delta\eta(z)X'(z)}{Y'(z)X(z) - Y(z)X'(z)}. \tag{24}$$

This gives a two-dimensional distribution of β_i^{stoch}. From this, we have to remove the space charge effects in a way very similar to what was done for F_{50}^{blur} in Eqs. (17)–(20). Finally, we can obtain the β_{50}^{MC} value, which should be compared with the $\beta_{50}^{\mathrm{blur}}$ obtained analytically. The spot size is given by $d_{50}^{\mathrm{blur}} = M\beta_{50}^{\mathrm{blur}}(z_{\mathrm{foc}})$, where d_{50} is the spot size into which 50% of all the particles fall.

As an example, we show here the results for a Ga focused-ion-beam system with a column voltage of 30 kV and an extraction voltage of 12 kV. The system has an accelerating lens at 10 mm ($V_1 = 55$ kV) and a decelerating lens at 300 mm ($V_2 = 10$ kV). The current is 1 nA and the system is at its optimum magnification of $M = 0.36$. From Fig. 7, we see that, without correction, the analytical calculation severely overestimates the Coulomb blurring. With correction, very good agreement is found between the analytical results and the Monte Carlo simulations.[13]

Another aspect that differs is that aperturing can reduce the Coulomb blurring in the Holtsmark regime. This is not what one would normally expect since $r''_{50H} \sim I'$, where $I' = I/\pi r_{\mathrm{beam}}^2$ is the current density, which does not change when passing through an aperture. The change in r'' is a direct result of the different r'' values for off-axis trajectories, an effect not taken into account in the theory of Jansen.[4] This can be clearly seen in Fig. 6. In the Holtsmark regime, i.e., $\lambda r_{\mathrm{beam}} \gg 1$, the correction value $C(\lambda r_{\mathrm{beam}})$ decreases when the aperture parameter a approaches unity. This is a result of the narrower probability distribution function at the edge of the beam. Therefore, after aperturing, the probe forming electrons are closer to the edge of the beam and thus the Coulomb blurring is smaller.

IV. CONCLUSIONS

We have shown that improved estimates of Coulomb blurring can be obtained by using a combination of numerical and analytical techniques. The theory is based on the numerical evaluation of probability distribution functions whose widths are used in the analytical evaluation of the Coulomb blurring. This leads to a correction factor $C(\lambda r_{\mathrm{beam}}, a)$ to the theory of Jansen.[4] Note that this depends only on $\lambda r_{\mathrm{beam}}$. This has the great advantage that the correction factor can be used as a simple interpolative function and does not need to be recalculated for every change of V, I, m, or r_{beam}. We have also included the effects of aperturing. This approach removes some of the deficiencies of the theory of Jansen,[4] especially in the intermediate regime. These result from inaccuracies in the interpolative scheme and the restriction to trajectories on the optical axis. We find good agreement with Monte Carlo simulations.

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[12] See, e.g., W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. *Numerical Recipes in Fortran* (Cambridge University Press, Cambridge, England, 1986).
[13] The small wiggles in β_{50}^{MC} are a result of the fact that in that region $Y'(z)X(z) - Y(z)X'(z)$ is very small and β_{50}^{MC} is difficult to determine.